

Subpixel Spatial Resolution of the X-Ray Charge-Coupled Device Based on the Charge Cloud Shape

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When an X-ray photon lands into a pixel (event pixel), the primary charge is mainly collected into the event pixel. If the X-ray landing position is sufficiently close to the pixel boundary, the primary charge spills over to the adjacent pixel forming split events. We can easily understand that there are three parameters coupled together; the X-ray landing position inside the pixel, the X-ray event pattern and the primary charge cloud shape. We can determine any one of them from the other two parameters. Since we know the charge cloud shape using the multi-pitch mesh experiment, we can calculate the X-ray landing position with subpixel resolution using the event pattern. We applied our method to Ti-K X-rays for the charge-coupled device with $12\mu\text{m}$ square pixel. Once the primary charge splits into the adjacent pixel, we can determine the X-ray landing position with subpixel resolution. Using three- or four-pixel split events, we can determine the X-ray landing position with an accuracy of less than $1\mu\text{m}$. For a two-pixel split event, we obtained a similar position accuracy in the split direction with no improvement in the direction perpendicular to it. We will discuss the type of CCD which can achieve the subpixel resolution for the entire area of the CCD.

Key words: charge-coupled device, X-ray event, split event, subpixel spatial resolution

1 Introduction

A charge-coupled device (CCD) is widely used in optical imaging, particularly in the digital camera for commercial use. It mainly employs an interline type CCD. The pixel size is approximately a few μm square which produces a few-mega-pixel image [1]. Although the interline type CCD has a relatively poor opening area, the micro-lens array system can increase the effective opening area up to 70% or higher. Furthermore, the CCD for optical region requires the depletion region to be at the most several μm . However, the CCD for X-ray use has different characteristics from that for optical use. It has a relatively good spatial resolution and a moderate energy resolution. Since the micro-lens array does not work for X-ray photons, the frame transfer type CCD is required for X-ray use to have a high opening area. The low energy X-ray, especially below 1 keV, is easily photoabsorbed, which requires the material above the depletion region to be as thin as possible. The cross-over of the gate structure above the depletion region makes the low energy X-ray responsivity within the pixel complicated. The photoabsorption depth in silicon for 10 keV X-ray is about 100 μm , which requires a much thicker depletion region for X-ray use than that for optical use.

Several CCDs for X-ray use, particularly for X-ray astronomy, have been developed to date. The ASCA satellite launched in February, 1993, employs CCDs with 27 μm square pixels with a depletion depth of 35 μm [2,3]. The Chandra Observatory launched in July, 1999, employs CCDs with 24 μm square pixels with a depletion depth of about 70 μm [4,5]. The XMM-Newton Observatory launched in December, 1999, employs two types of CCDs [6]: one has a 150 μm square pixel with a depletion depth of 280 μm [7] while the other has a 40 μm square pixel with a depletion depth of 40 μm [8]. These CCDs for X-ray use are developed to have thick depletion regions rather than to have high spatial resolution.

When an X-ray photon is photoabsorbed in a CCD, it generates a number of electrons proportional to the incident X-ray energy. The electrons generated by X-ray photons usually expand by the diffusion process while they are pulled to the potential well of the CCD pixel. They usually form a charge cloud of a finite size. They are collected into several pixels forming various types of event pattern ('grade') depending on how they split. When the entire charge is collected into one pixel (no surrounding pixels have a signal), it is called a 'single pixel event': when it splits into more than one pixel, it is called a 'split pixel event'. The event grade is determined both by the landing position of X-rays within the pixel and by the charge cloud shape. The X-ray responsivity depends on the event grade as well as its landing position. This is quite in contrast to the optical photon that generates only one or two electrons. Therefore, there is no concept of the event grade in an optical region.

We introduced a new technique, ‘mesh experiment’, which enables us to measure the X-ray responsivity of the CCD with subpixel resolution [9]. In this experiment, a parallel X-ray beam is irradiated onto the CCD chip above which a metal mesh is placed. The mesh has many small holes which are periodically spaced. There are two types of experiments; a single pitch mesh experiment and a multi-pitch mesh experiment. If the small hole spacing on the mesh is equal to the CCD pixel size, it is called a single pitch mesh experiment and if it is a multiple of the CCD pixel size, it is called a multi-pitch mesh experiment. Using this technique, the detailed gate structures were directly measured from the X-ray absorption feature [10,11]. The details of the mesh experiment are described in literature by Tsunemi et al. [12]

Using the multi-pitch mesh experiment, we can unequivocally identify the X-ray landing position inside the pixel. In this way, we can directly measure the event grade, and how the charge cloud splits into surrounding pixels, as a function of the landing position inside the pixel. We can find out that the fraction of the charge splitting into the adjacent pixel increases as the X-ray landing position approaches the pixel boundary. We can easily understand that there are three parameters coupled together; the X-ray landing position inside the pixel, the X-ray event grade and the charge cloud shape. If we know two out of three parameters, we can calculate the third one. The X-ray event grade is easily measured by the photon count CCD system. The X-ray landing position can be directly measured by the mesh experiment, resulting us to measure the charge cloud shape [13]. Once we know the charge cloud shape, we can measure the X-ray landing position without applying the mesh experiment.

In this paper, we briefly describe the mesh experiment and present the method of determining the X-ray landing position for various types of event grades in order to achieve the subpixel resolution.

2 Experiment

An X-ray photon photoabsorbed inside the CCD usually generates a number of electrons, the primary charge cloud. One X-ray photon photoabsorbed generates one X-ray event, a series of pixels collecting a primary charge cloud. The primary charge cloud expands to some extent while it is pulled to the potential well. If the X-ray photon is photoabsorbed below the depletion region, some fraction of the charge is collected as a multi-pixel event. If the X-ray photon is photoabsorbed in the depletion region, the size of the primary charge cloud is at the most a few μm which is smaller than that of the CCD pixel size. The actual charge cloud size depends on the photoabsorbed depth. Therefore, we can distinguish the events photoabsorbed in the depletion region from those

photoabsorbed below the depletion region by the event pattern. The former shows the incident X-ray energy while the latter does not due to the charge loss. We will focus on the events photoabsorbed in the depletion region.

We will obtain various grades of events depending on the X-ray landing position. A major fraction of the primary charge will be collected in the pixel in which the X-ray lands. We term this pixel as the ‘event pixel’. When the entire primary charge cloud is collected into the event pixel, the surrounding pixels have no signal, resulting in a single pixel event. If the X-ray landing position in the event pixel is sufficiently close to the pixel boundary, the primary charge splits into two pixels forming a two-pixel split event. If the X-ray landing position is close to the event pixel corner, the primary charge splits into three or four pixels forming three- or four-pixel split event or ‘corner event’.

When we detect an X-ray event in the CCD, we usually see 3×3 pixels as the event pattern. The central pixel of the event pattern is the event pixel that has the maximum charge in the 3×3 pixels. The pixels around the event pixel are ‘surrounding pixels’. In practice, we introduce the split threshold level, T_h , in order to test whether or not the pixel has charge. If we find that the output from the surrounding pixels exceeds T_h , we term the pixel as a ‘split pixel’. In X-ray spectroscopy, we usually sum up the output from the event pixel and those from the split pixels in order to evaluate the incident X-ray energy. Since each pixel usually contains noise level, the best energy resolution is obtained by eliminating the pixels whose output is less than T_h . The overall noise level in our system is 10 electrons or less, therefore, we set T_h to be 50 electrons so that we do not treat the pixel with no signal as a split pixel by noise.

We performed the mesh experiment employing a CCD (Hamamatsu Photonics, N38 11-5A0N-2) consisting of $12\mu\text{m}$ square pixels for X-ray use. The mesh fabricated of gold has small holes of $2.1\mu\text{m}$ diameter spaced $48\mu\text{m}$ apart. The pitch of mesh holes is four times larger than the CCD pixel size which forms a multi-pitch mesh experiment. The mesh is placed just 1 mm above the CCD. In this way, we can measure what type of event grades are generated as a function of the X-ray landing position inside the CCD pixel.

3 Event Pattern

When an X-ray photon lands on the CCD at (X_{in}, Y_{in}) , the output, $D(n, m; X_{in}, Y_{in})$, from the (n, m) pixel in the X-ray event is expressed as an integration of the primary charge cloud, $C(X, Y)$, over the pixel area that

is given in eq. (1).

$$D(n, m; X_{in}, Y_{in}) = \int_{X_n}^{X_{n+1}} dX \int_{Y_m}^{Y_{m+1}} dY C(X - X_{in}, Y - Y_{in}) \quad (1)$$

where X_n, X_{n+1} , and Y_m, Y_{m+1} represent the pixel boundary of the X and Y coordinates, respectively. Since the CCD employed has a square shaped pixel, we set $X_{n+1} - X_n = Y_{m+1} - Y_m \equiv L$, where L represents the pixel size. We assume that all the CCD pixels are identical, therefore, we obtain the relationship in eq. (2) as below,

$$D(n + k, m + l; X_{in}, Y_{in}) = D(n, m; X_{in} - k L, Y_{in} - l L) . \quad (2)$$

When the (n, m) pixel represents the event pixel, the event pattern of the 3×3 pixels are expressed in the matrix below,

$$\begin{pmatrix} D(n-1, m+1; X_{in}, Y_{in}) & D(n, m+1; X_{in}, Y_{in}) & D(n+1, m+1; X_{in}, Y_{in}) \\ D(n-1, m; X_{in}, Y_{in}) & D(n, m; X_{in}, Y_{in}) & D(n+1, m; X_{in}, Y_{in}) \\ D(n-1, m-1; X_{in}, Y_{in}) & D(n, m-1; X_{in}, Y_{in}) & D(n+1, m-1; X_{in}, Y_{in}) \end{pmatrix} \quad (3)$$

It can be rewritten in the form below using eq. (2) as,

$$\begin{pmatrix} D(n, m; X_{in} + L, Y_{in} - L) & D(n, m; X_{in}, Y_{in} - L) & D(n, m; X_{in} - L, Y_{in} - L) \\ D(n, m; X_{in} + L, Y_{in}) & D(n, m; X_{in}, Y_{in}) & D(n, m; X_{in} - L, Y_{in}) \\ D(n, m; X_{in} + L, Y_{in} + L) & D(n, m; X_{in}, Y_{in} + L) & D(n, m; X_{in} - L, Y_{in} + L) \end{pmatrix} \quad (4)$$

In this way, the 3×3 pixel data express the function of D . Employing the multi-pitch mesh experiment, we can directly measure the 3×3 pixel data as a function of (X_{in}, Y_{in}) . Then, we can obtain the function, D , which is expressed as D_n in the literature [13], from the raw data. In practice, we relocate the event pattern to match the function, D in eq. (1), which is shown in Fig. 1 in 3×3 pixel region.

Using the eq. (1), we find that the charge cloud shape is obtained by differentiating D with (X_{in}, Y_{in}) . The detailed derivation of the charge cloud shape is given in the literature [13]. In the mesh experiment, we can confine the X-ray landing position with the precision of the mesh hole. Therefore, the differentiation of D is a convolution between the charge cloud shape and the mesh hole shape. Since we know the mesh hole shape, we can deduce the actual

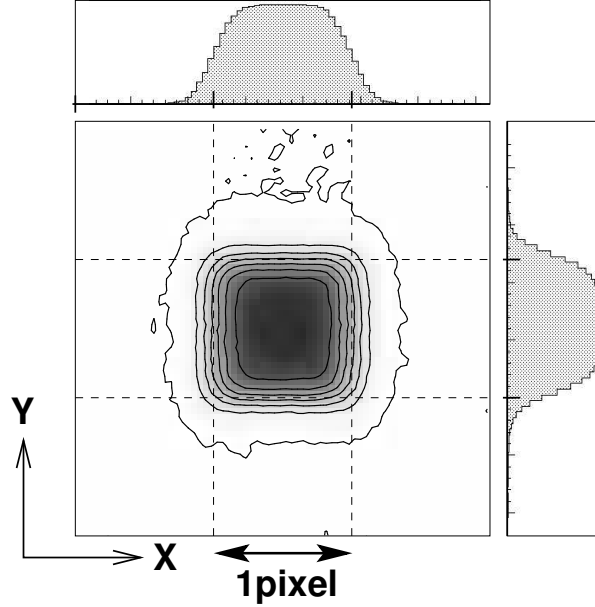


Fig. 1. Signal output from the event pixel as a function of the X-ray landing position in the 3×3 pixel region. Projections along X and Y axes are also shown.

charge cloud shape which is well approximated by an axial symmetric Gaussian function. In this way, we can calculate the primary charge cloud shape as a function of the incident X-ray energy as shown in Fig. 2 [14].

The longer the attenuation length of X-ray photons in silicon, the bigger is the charge cloud size. This is well approximated by a simple diffusion model [15]. In the following analysis, we will mainly focus on the Ti-K X-ray photons since it has the biggest charge cloud size in our analysis. Then, we will estimate the X-ray landing position by comparing the event pattern with D .

4 Data Reduction

4.1 Analysis method

Once we know the charge cloud shape, we need not employ the mesh any more. Since we can easily determine the X-ray event pattern, we can calculate the incident X-ray energy by adding up the signal contained in the event. Then we can estimate the charge cloud shape and calculate D according to eq. (1).

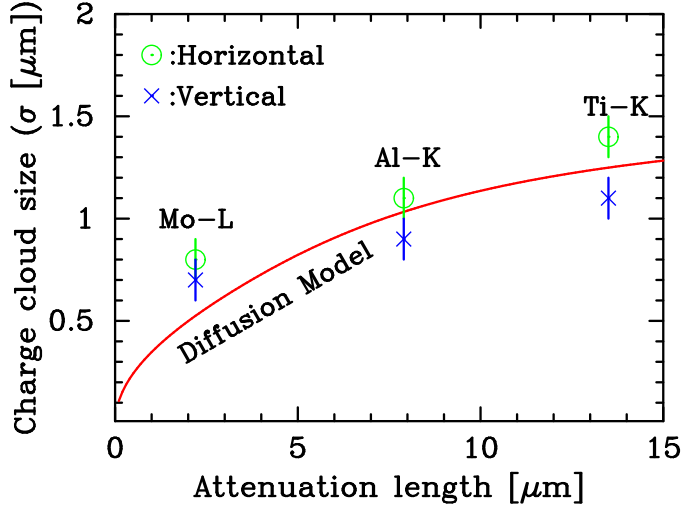


Fig. 2. Primary charge cloud size generated by various X-ray photons for Mo-L (2.3 keV), Al-K (1.5 keV) and Ti-K (4.5 keV) as a function of the attenuation length in silicon. The solid line represents the model calculation.

Figure 3 shows D which is free from the effect of the mesh hole shape.

When we obtain a 3×3 event pattern, we can compare it with the eq. (4). We calculate the sum of the square of differences between the 3×3 pixel data and D as a function of (X_{in}, Y_{in}) . The estimated landing position is given as the position when the sum is minimum. Once we detect an X-ray event, we always employ the 3×3 pixel data regardless of its grade, whether it is a single pixel event or not etc. It should be noted that our method does not take into account T_h . However, we will sort the event by grades to determine which grades can yield how much accuracy in estimating the landing position.

4.2 Estimated landing position

Using this method, we can evaluate the X-ray landing position, (X_{in}, Y_{in}) , while we know the location of the mesh hole shadow on the CCD, (X_{hole}, Y_{hole}) , in which the X-ray must have landed. Then the difference, $\Delta \equiv (X_{in}, Y_{in}) - (X_{hole}, Y_{hole})$, shows the uncertainty of the position estimation. We calculate Δ for all X-ray events to estimate the position accuracy. Since the actual landing position of the X-ray photon is somewhere inside the mesh hole, Δ is a convolution between the mesh hole shape and the uncertainty of the estimation of the X-ray landing position.

Figure 4 shows the distribution of Δ for various event grades. In this figure, we plotted the distribution of Δ in the $24 \mu\text{m}$ square. The mesh hole shadow

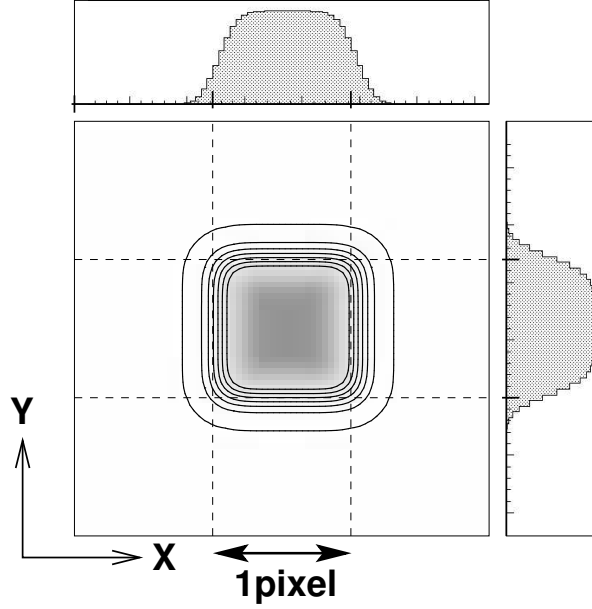


Fig. 3. Model calculation for D . The signal output from the event pixel is shown as a function of the X-ray landing position in the 3×3 pixel region. This figure is free from the effect of the mesh hole shape.

is also shown by the small circle on the lower left side of the figures and the dashed squares represent the size of the CCD pixel for comparison. We fitted the results by two-dimensional Gaussian function and obtained the size of the major and minor axes. The major and minor axes always coincide with the horizontal or vertical directions on the CCD. It should be noted that Fig. 4 denotes the actual position accuracy convoluted with the mesh hole shape. The geometrical mesh hole size is $2.1 \mu\text{m}$ in diameter while the effective mesh hole shadow on the CCD is expanded by the diffraction. The actual mesh hole shadow on the CCD is about $2.2 \mu\text{m}$ for Ti-K X-rays in our configuration. Hence we can eliminate the effect of the mesh hole shape to evaluate the position accuracy of our method summarized in Table 1.

For single pixel events, only one pixel contains a significant fraction of the charge while the surrounding pixels contain noise. Therefore, the landing position inside the pixel is well within the pixel boundary where D is almost constant. The actual shape of the region where the single pixel event is generated is well within the pixel boundary. The position uncertainty is slightly better than the pixel size.

The position accuracy can be improved when the charge splits into adjacent

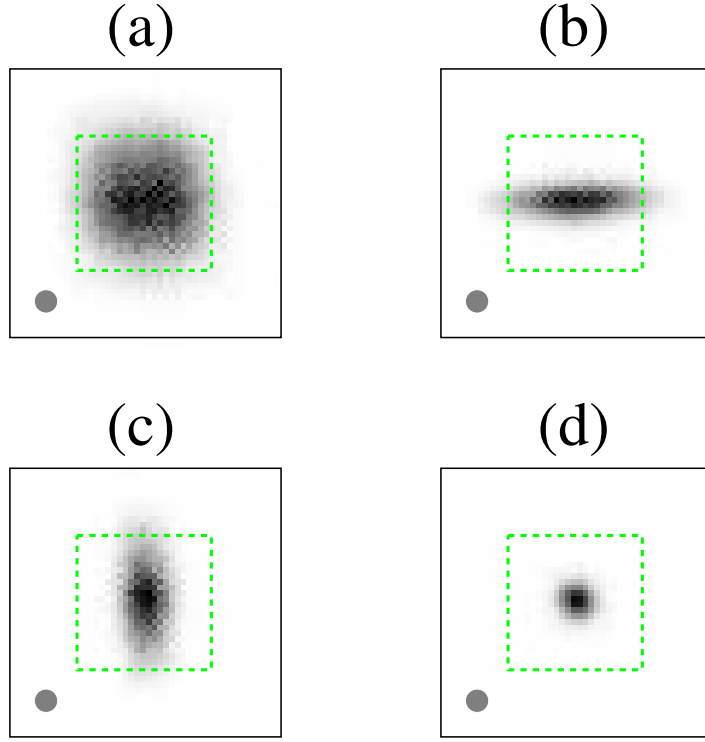


Fig. 4. Position accuracies using our method shown in a $24\mu\text{m}$ square. The small circle in the lower left shows the shape of the mesh hole shadow on the CCD and the dashed square represents the size of the CCD pixel. Position accuracy for single pixel events (a), for vertically split two-pixel events (b), for horizontally split two-pixel events (c) and for corner events (d).

pixels. When the X-ray landing position is sufficiently close to the vertical boundary, the X-ray event forms a horizontally split two-pixel event. In this case, the X-ray landing position can be improved along the horizontal direction. However, there is almost no improvement in the vertical direction. A similar improvement can be achieved for a vertically split two-pixel event. We note that the position accuracy of split direction for the vertically split two-pixel event is better than that of the horizontally split two-pixel event. The smaller extent of the charge cloud has higher electron density than the bigger extent of the charge cloud. The higher electron density will lead to a finer position accuracy. Therefore, the above fact is consistent with the elongation of the charge cloud shape [14]. Finally, when an X-ray lands near the pixel corner, the charge splits both along the horizontal and the vertical directions. Then we can improve the two-dimensional position resolution.

Yoshita et al. [16] have already demonstrated that the CCD has a subpixel spatial resolution using split events. They obtained the position accuracy to $1.5 \sim 2.0\mu\text{m}$. However, they employed only two-pixel split events, resulting in the improvement of the position resolution for one dimension. This is mainly

due to the experimental setup: they employed a single pitch mesh experiment. They had difficulties in precisely determining the X-ray landing position for corner events. However, we employed a multi-pitch mesh experiment by which we could unequivocally determine the X-ray landing position for all X-ray events. Hence, we could improve the two-dimensional position resolution for the first time. Furthermore, we introduced the mesh with smaller holes to improve the position accuracy.

4.3 Position estimation using the event pixel

This is a very conventional method where the center of the event pixel is considered to be the X-ray landing position. The position accuracy using this method should be determined by the convolution between the pixel shape and the mesh hole shadow. If we assume that the X-ray detection efficiency is uniform over the pixel, we can calculate the position accuracy which is $3.6\ \mu\text{m}$ (standard deviation, σ) using $12\ \mu\text{m}$ square pixels and $2.2\ \mu\text{m}$ diameter mesh holes. We evaluated the accuracy of the position estimation employing this conventional method. Figure 5 shows the distribution of Δ using all the X-ray events. We will analyze the result by the same method used in our study. The results listed in Table 1 are almost consistent with what we expected. A small difference between our results and those we expected is probably due to the nonuniformity of the X-ray detection efficiency over the pixel.

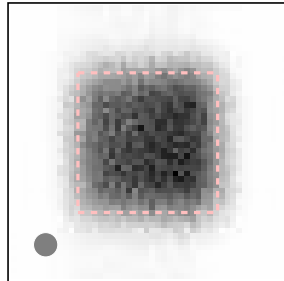


Fig. 5. Same as for Fig.4 using the center of the event pixel as the X-ray landing position.

5 Discussion

So far, the spatial resolution of the CCD is considered to be limited by the pixel size. Furthermore, the charge cloud generated by X-ray photons expands,

Table 1
Accuracy of the incident X-ray position

Ti-K X-rays	Branching ratio	Horizontal direction	Vertical direction
	(%)	(μm)	(μm)
Single pixel event	55.2	3.1 ± 0.2	3.4 ± 0.2
Horizontally split two-pixel event	20.3	1.0 ± 0.1	3.1 ± 0.2
Vertically split two-pixel event	13.0	3.4 ± 0.2	0.6 ± 0.1
Corner event	11.5	0.7 ± 0.1	0.7 ± 0.1
Event pixel		3.4 ± 0.2	3.9 ± 0.2

resulting in the incident X-ray position blur.

By the conventional method, the position accuracy (σ) determined by the pixel size would be approximately 0.3 times of the pixel size. Tsunemi et al. [12] reported a method to improve the position accuracy up to 0.13 times of the pixel size. They estimated the X-ray landing position by employing the center of gravity of the X-ray event pattern, particularly for the two-pixel split events. However, the center of gravity of the event does not precisely show the X-ray landing position since the charge cloud size is smaller than the pixel size. The precise X-ray landing position should be determined by referring to the charge cloud shape. Therefore, our method, considering the charge cloud shape, can improve the accuracy of the X-ray landing position better than that using the center of gravity. Our result shows the accuracy of the X-ray landing position up to 0.06 times the pixel size, which shows that the CCD for X-ray use can be an image sensor with a sub μm resolution.

The charge cloud size of the X-ray used in our experiment is relatively small compared with the CCD pixel size employed. This combination makes the fraction of the single pixel event high and that of the split event, particularly the corner event, low as described in Table 1. The improvement of the position resolution can be effectively attained when the charge splits into the adjacent pixel. Since our method is practically useful only for corner events, we have to increase the fraction of the split events in order to make the entire area of the X-ray CCD as an image sensor with a sub μm resolution. What are the practical conditions by which we can obtain the subpixel resolution using our method more effectively? There are two ways to do this: one is to make the charge cloud size big and the other is to manufacture a CCD chip with small pixel size.

The charge cloud shape depends on the travel distance between the photoabsorption location and the potential well. The longer the travel distance, the bigger is the charge cloud shape. Since the CCD employed is a front illumination type (FI) CCD, the travel distance becomes longer for higher X-ray

energy, resulting in a bigger charge cloud shape. However, this does not apply to a back illumination type (BI) CCD. In the BI CCD, the X-ray photon enters from behind the depletion region. X-rays with shorter photoabsorption length generate a charge cloud at the far end of the depletion region. The charge cloud will travel a relatively long distance, resulting in a relatively large cloud shape. Therefore, a low energy X-ray in the BI CCD will generate a larger charge cloud than that in the FI CCD. Our method will function efficiently in the BI CCD.

The accuracy of the X-ray landing position depends on the accuracy of the charge cloud shape. The actual charge cloud shape will depend on various parameters; the incident X-ray energy, the thickness of the depletion region and the working condition of the CCD, and the applied voltage on the gates and the clocking pattern. We can directly measure the charge cloud shape using the mesh experiment. However, obtained the charge cloud shape is a mean shape for a given X-ray energy, it will be different for individual X-ray photons depending on the photoabsorption depth. This will become a position error through our method.

Our method requires the charge cloud generated by the X-ray photon to spill over the adjacent pixel. Therefore, we need not make the CCD pixel very small if the pixel size is comparable to the primary charge cloud size. Furthermore, we need a CCD with a thicker depletion region to obtain a higher detection efficiency for high energy X-ray. We only require the pixel size to be small enough to generate split events. What types of grades generated by an X-ray photon depend not only on where the X-ray lands but also on how deep the X-ray is photoabsorbed in the depletion layer which is a stochastic process. The charge cloud size (σ) measured for Ti-K(4.5 keV) X-rays is $1.0 \sim 1.4 \mu\text{m}$. Considering the noise level, we can detect the split charge to the adjacent pixel when the X-ray photon lands within about $3 \mu\text{m}$ away from the boundary. Therefore if the pixel size is about $6 \mu\text{m}$ square, we can obtain split events wherever the X-ray lands. In the present CCD, having $12 \mu\text{m}$ square pixel, X-rays landing on the central part of the pixel become single pixel events even if they are photoabsorbed deep in the depletion region.

We should note that the X-ray photoabsorbed in the shallow region generates a very small charge cloud size in the FI CCD. Therefore, some fraction of X-ray photons generates single pixel event however small the pixel size is. Whereas no X-ray photon landing onto the central part of the pixel generates a split pixel event if the pixel size is bigger than the charge extent. The branching ratio of the X-ray events does not represent the area generating each event grade but represents what fraction of the X-ray events becomes what type of grades. Hence, we can expect that some X-ray events will generate split events even if they land at the center of the pixel of the CCD with about $6 \mu\text{m}$ square pixel. Since the CCD chip employed at present has a $12\text{-}\mu\text{m}$ -square pixel, we

can say that the CCD with two times smaller pixel will be an image sensor with a sub μm resolution.

6 Conclusion

We performed the multi-pitch mesh experiment using the gold mesh of $2.1\ \mu\text{m}$ diameter holes. Then, we calculated the function, D , which shows the output from the event pixel as a function of the X-ray landing position. The primary charge cloud shape generated by X-ray photons can be measured from D .

Using the charge cloud shape, we can calculate the X-ray landing position with subpixel resolution. Our method compares the 3×3 pixel data with D . The position resolution is improved in the direction where the charge splits. Therefore, there is almost no improvement for single pixel events. The position resolution for two-pixel split events can be improved in one direction. When the X-ray photon lands near the pixel corner, the charge splits both in the horizontal direction and the vertical direction generating corner events. Then the two-dimensional position resolution can be improved to subpixel resolution. The accuracy of the position is less than $1\ \mu\text{m}$ in the direction where the charge splits.

We have discussed how we can improve the position resolution of the CCD for X-ray use by introducing our method. Our method becomes practical when an X-ray photon produces a split event. For the optical region, a CCD with very small pixel size is manufactured whereas it is not designed for X-ray use. Taking into account the noise level in our system, we find that the CCD with a pixel size of about $6\ \mu\text{m}$ square will generate split events from the entire region. Therefore, the CCD can be used as an image sensor with a sub μm resolution for X-ray photons.

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